Small T_1^{-1} coherence peak near T_c in unconventional BCS superconductors

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It is usually believed that a coherence peak just below T_c in the nuclear spin lattice relaxation rate T_1^{-1} in superconducting materials is a signature of conventional s-wave pairing. In this paper we demonstrate that **any** unconventional superconductor obeying BCS pure-case weak-coupling theory should show a small T_1^{-1} coherence peak near T_c, generally with a height between 3 and 15 percent greater than the normal state T_1^{-1} at T_c. It is largely due to impurity and magnetic effects that this peak has not commonly been observed.

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It is well known [1] that conventional superconductors obeying BCS weak-coupling theory generally show a large coherence peak in the nuclear spin lattice relaxation rate T_1^{-1} below T_c. This is a direct consequence of the large quasi-particle density-of-states found for $E \geq 1.0$ at the gap edge. It is commonly believed, and experimentally largely true, that unconventional superconductors show no coherence peak near T_c. However, a simple quantitative argument shows that if the BCS weak-coupling pure case theory applies, a small coherence peak below T_c must exist.

Consider the BCS weak-coupling equation for the nuclear spin lattice relaxation rate T_1^{-1} for unconventional superconductors:

$$(T_1T)^{-1}/(T_1T)^{-1}_{|T=T_c} = \int_0^\infty dE\, N^2(E)\mathrm{sech}^2(E/(2T))/2T \qquad (1)$$

The $\mathrm{sech}^2(E/(2T))$ acts as an attenuation factor and dominates the low-temperature T_1^{-1}, yielding exponentially activated behavior for s-wave superconductivity and power-law behavior for unconventional superconductivity. However, as $T \to T_c$ all of the structure in N(E) (i.e. DOS different from unity) is shifted to lower energies, since $N(E) = N(E/\Delta)$ and $\Delta \to 0$. See Figure 1 for a depiction of this behavior for the 3-d ^{3}-He A-phase order parameter $\Delta(\mathbf{k}) = \Delta \sin\theta$. All of the structure in N(E) falls in the region where $E/2T \ll 1$, so that for this structure the exponential damping factor becomes essentially irrelevant. Define $F(E) = N(E) - 1$. Note that by the density-of-states sum rule, $\int_0^\infty F(E)dE = 0$. Now substituting in for N(E) we find

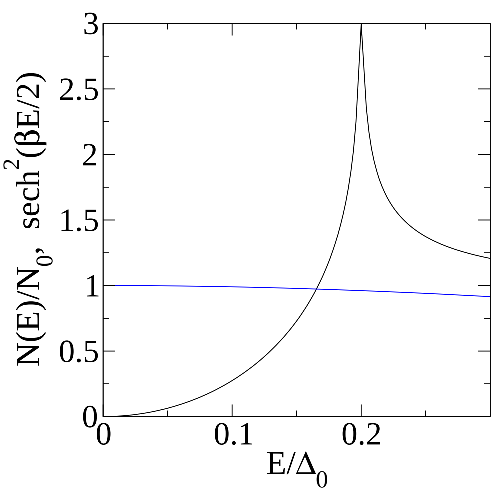

FIG. 1: Diagram depicting attenuation factor and quasi-particle density-of-states for $T \simeq 0.98T_c \simeq 0.5\Delta_0, \Delta = 0.2\Delta_0$, 3-d ^{3}-He A-phase order parameter.

$$(T_1T)^{-1}/(T_1T)^{-1}_{|T=T_c} = \int_0^\infty dE(1+2F(E)+F^2(E))\mathrm{sech}^2(E/(2T))/2T \qquad (2)$$

The first term trivially yields 1. The second term, $\int_0^\infty dE\ 2F(E)\mathrm{sech}^2(E/(2T))/2T$ can be evaluated by noticing that as $\Delta \to 0$, F(E) is only significantly different from 0 in regions where the argument of the sech^2 is small, so that to an excellent approximation near T_c this integral is equal to $\int_0^\infty F(E)\,dE = 0$. The final term, $\int_0^\infty dE\, F^2(E)\mathrm{sech}^2(E/(2T))/2T$, is positive, and so in the immediate neighborhood of T_c, $(T_1T)^{-1}/(T_1T)^{-1}_{|T=T_c} > 1$, implying the existence of a peak. It is this redistribution of N(E) away from an energy-constant ($= N_0$) density-of-states, represented by $F^2(E)$, that is responsible for the peak in T_1^{-1} near T_c. The larger this effect, the larger the peak.

This redistribution is intimately tied in with the nodal structure of $\Delta(\mathbf{k})$. This can be seen directly from the BCS expression for the density-of-states $N(E/\Delta) \equiv N(x) = \mathrm{Re}\langle\frac{x}{\sqrt{x^2-f^2}}\rangle$, where $\langle\ldots\rangle$ denotes an average over the Fermi surface and f contains the angular dependence of the order parameter. (i.e., $\Delta(\mathbf{k}) = \Delta_0 f(\mathbf{k})$). The contribution of the nodes is most easily parametrized by $< f^2 >$, with larger values indicating less nodal order parameters. For example, an s-wave order parameter has $< f^2 > = 1$, while a 2d d-wave order parameter (containing line nodes) has $< f^2 > =0.5$. Gap functions f with larger $< f^2 >$, indicating effectively small or absent nodes, have a comparatively smaller region of phase space contributing to the integral, for $x < 1$. These gap functions will therefore show depleted low-energy density-of-states, and by the sum rule must have enhanced spectral weight in the peak at $E = \Delta$. Both effects will tend to enhance the T_1^{-1} peak just below T_c.

These behaviors are illustrated in Figure 2, which depicts densities-of-states and T_1^{-1} for a series of 3-d order parameters $\Delta(\mathbf{k}) = 1 - \cos^n(\theta)$, with θ the polar angle. As n increases, the low-energy DOS is depleted and the coherence-peak DOS enhanced, with a concomitant increase in the T_1^{-1} peak near T_c. For these cases, $< f^2 >$ increases monotonically from $\frac{8}{15} \simeq 0.533$ for n=2 to 0.866 for n=10.

Results.- In Figure 3 are depicted the coherence peaks near T_c for several unconventional order parameters: $d_{x^2-y^2}$-wave, the ^{3}-He A-phase order parameter (for which $\Delta(\mathbf{k}) = \Delta_0 \sin\theta$), and the p-wave 3-dimensional order parameter $\Delta(\mathbf{k}) = \Delta_0 \cos\theta$, as well as the quasiparticle density-of-states for these order parameters. Note that a small peak just below T_c is evident even for the last order parameter, whose quasiparticle density-of-states shows no divergence at $E = \Delta$. The

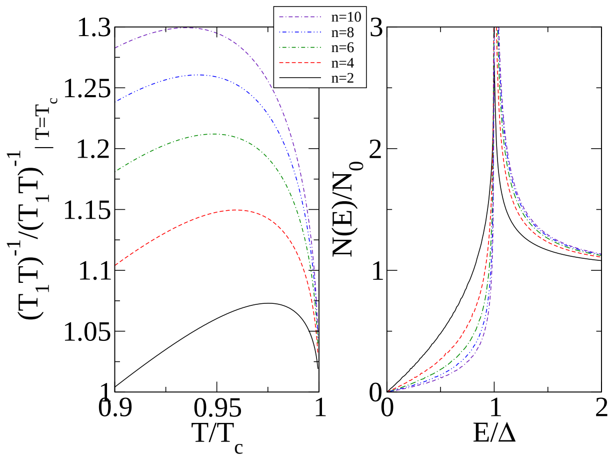

FIG. 2: The densities-of-states and T_1^{-1} for several 3D order parameters $\Delta(\mathbf{k}) = 1 - \cos^n(\theta)$ are shown.

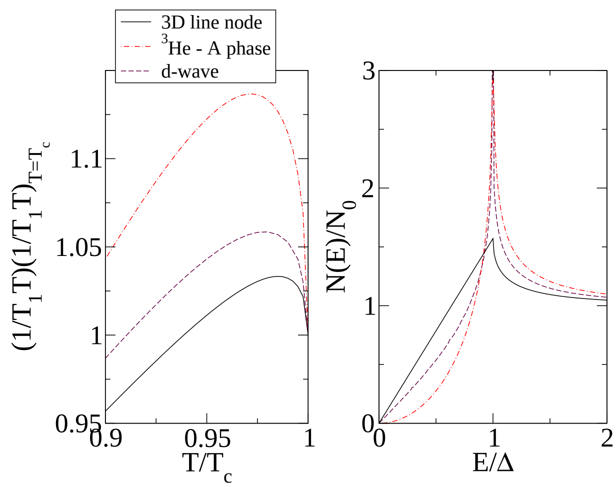

FIG. 3: The predicted nuclear spin lattice relaxation rates $(T_1 T)^{-1}$ near T_c and quasiparticle densities-of-states are shown for three order parameters: 2D d-wave, the A phase of ^3He, and a 3D line-node model.

analysis of the preceding paragraph demonstrates that it is largely the second moment of the DOS around an energy-constant DOS ($\simeq N_0$) that produces the small peak just below T_c. While a large or divergent DOS at $E = \Delta$ clearly enhances the coherence peak near T_c, it is not necessary for the formation of a peak.

For the three cases described above, it is possible to derive an analytic expression for T_1^{-1} just below T_c and compare with the numerical results. The quasiparticle density-of-states for each of the three order parameters can be computed analytically, and one finds the following well known results [2, 3, 4], where $x = E/\Delta$ and K is the elliptical function:

$$\begin{aligned}
\mathrm{d-wave}: N(x) &= \frac{2}{\pi} K(\frac{1}{x}), x < 1; && (3)\\
&= \frac{2}{\pi} x K(x), x > 1 && (4)\\
{}^3\mathrm{He\ A-phase}: N(x) &= \frac{x}{2}\log(|\frac{1+x}{1-x}|) && (5)\\
\mathrm{3d-linenode}: N(x) &= \frac{\pi}{2} x, x \leq 1; && (6)\\
&= x \sin^{-1}(\frac{1}{x}), x \geq 1. && (7)
\end{aligned}$$

Now, to work out an analytic form for the peak in T_1^{-1} just below T_c, we must compute $\int_0^\infty dE F^2(E) \mathrm{sech}^2(E/(2T))/2T$, where $F(E) = N(E) - 1$. For T sufficiently near T_c, F(E) only varies from zero in a region where $\mathrm{sech}^2(E/2T)$ is essentially unity, as described at the beginning of this paper. Making the substitution $E = \Delta x$, and taking $\mathrm{sech}^2(E/2T)$ as 1, we find for the above integrals, where γ is the Catalan constant= $0.915\ldots$

$$\begin{aligned}
\mathrm{d-wave}: &\simeq 0.4743\Delta/2T && (8)\\
{}^3\mathrm{-HeA-phase}: \frac{\pi^2}{12}\Delta/2T &\simeq 0.822\Delta/2T && (9)\\
\mathrm{3D\ line\ node}: (\frac{2}{3}\gamma - \frac{1}{3})\Delta/2T &\simeq 0.2773\Delta/2T && (10)
\end{aligned}$$

In other words, very near T_c ($T > 0.995T_c$) we can express the ratio $(T_1T)^{-1}/(T_1T)^{-1}_{|T=T_c}$ as simply $1+\alpha\Delta(T)/T$, where α is an order parameter-dependent constant, and this expression yields reasonably good agreement with the numerical results. In order to better model the behavior near T_c we have calculated analytically the next order term and found excellent agreement, as indicated in the plot below. Below 0.98 T_c this approximation becomes less accurate.

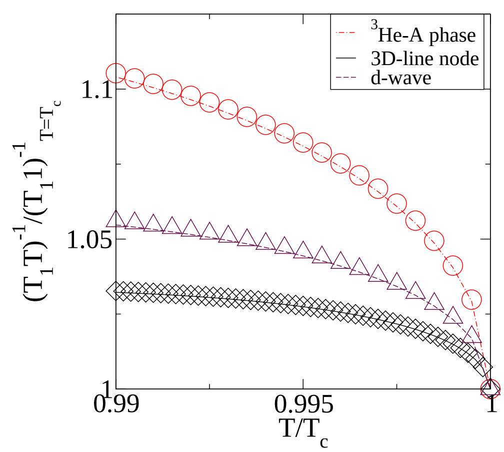

FIG. 4: The analytic and numerically computed T_1^{-1} for the three order parameters previously discussed are shown. Symbols indicate the analytic result and the lines the numerical result.

Discussion.- The foregoing analysis shows that BCS weak-coupling pure-case unconventional superconductors should exhibit a small T_1^{-1} coherence peak just below T_c. Yet a literature survey on this topic [6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27] has uncovered just two materials - $CePt_3Si$ and $(TMTSF)_2PF_6$-which show such a peak. The question therefore arises as to why such peaks are not commonly observed.

To address this question, we have conducted an analysis of the effect of resonant impurity scattering upon this T_1^{-1} peak, for a two dimensional d-wave order parameter. It is well known that such impurity scattering truncates the DOS peak at $E = \Delta$ and in addition can generate substantial low-energy density-of-states. Both of these effects would tend to reduce the size of the coherence peak. It turns out that for these reasons the appearance of this peak is extraordinarily sensitive to impurity scattering. Depicted below are four T_1^{-1} curves for d-wave superconductivity: zero impurity scattering, and three cases of small impurity scattering: $\Gamma/\Delta_{00} = 0.01$, 0.02 and 0.03. Within the unitary limit this last concentration is roughly 7 percent of the critical impurity concentration required to destroy superconductivity [28], and would result in a depression of T_c of this order. As is clear from the plot, the height of the peak is greatly diminished even by the rather low impurity scattering [3] rates modeled here.

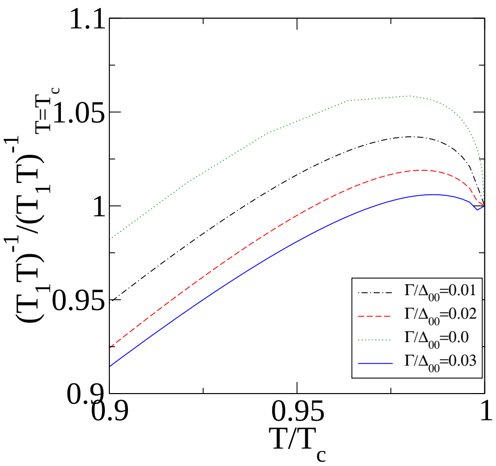

FIG. 5: The numerically computed T_1^{-1} for no impurity scattering, and for Γ/Δ_{00} = 0.01, 0.02 and 0.03 are shown.

Given that materials in the unitary limit typically have superconductivity destroyed by an impurity concentration on the order of a few percent [29], the foregoing analysis indicates that an impurity concentration of just 0.25 percent is sufficient to largely destroy this peak. Such a concentration is well within the range of observation [30].

In order to observe this peak samples of the highest possible quality are clearly essential, with impurity concentration less than 0.1 percent. It would also be advantageous to perform low-temperature specific heat measurements on the same samples as this would allow accurate assessment of the prediction of a finite relaxation rate at T=0, via a measurement of the residual density of states.

An additional effect complicating the observance of this peak is the frequent occurrence of magnetism in the heavy-fermion and high-T_c cuprate materials upon which most of the measurements have been performed. The combination of magnetism and the extreme sensitivity of this peak to the presence of impurities in the unitary limit make its observation difficult in the heavy-fermion and cuprate superconductors. However, the recently discovered non-centrosymmetric superconductor Li_2Pt_3B [31] shows no signs of magnetism or strong electron correlation [32], and appears to be unconventional on at least one band, based upon magnetic penetration depth data [32]. This material may therefore be an ideal material in which to search for this small T_1^{-1} peak. Another possibility for experiment is the class of organic superconductors, which may not necessarily have the sensitivity to impurities characteristic of the heavy-fermion and cuprate materials. Indeed, the organic superconductor $(TMTSF)_2PF_6$ has already shown a small peak below T_c [27].

To summarize, here we have demonstrated that any unconventional superconductor obeying BCS pure-case theory should show a small coherence peak in the nuclear spin lattice relaxation rate T_1^{-1} just below T_c. It is likely due to magnetic and impurity effects that this peak has not generally been observed in unconventional superconductors.

Acknowledgment

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